

Nonlinear current response of an isolated system of interacting fermions

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Nonlinear real-time response of interacting particles is studied on the example of a one-dimensional tight-binding model of spinless fermions driven by electric field. Using equations of motion and numerical methods we show that for a non-integrable case at finite temperatures the major effect of nonlinearity can be taken into account within the linear response formalism extended by a renormalization of the kinetic energy due to the Joule heating. On the other hand, integrable systems show on constant driving a different universality with a damped oscillating current whereby the frequency is related but not equal to the Bloch oscillations.

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Despite its importance for various branches of physics, the real-time response of quantum systems remains in many aspects an unexplored field. Only recently have the time-resolved measurements provided important information on the nonequilibrium short-time dynamics of correlated bulk materials [1] nanostructures [2] and optical lattice systems [3]. In contrast to the developments in the experimental methods, theoretical description of the real-time dynamics remains a difficult and challenging task. As the exact time evolution is known only for very few models (see the discussion in Ref. [4]), most of unbiased results has been obtained from advanced numerical approaches like exact diagonalization (ED) [5], time-dependent density matrix renormalization group (tDMRG) [6] or nonequilibrium dynamical mean-field theory (nDMFT) [7]. These approaches allow for studying various phenomena, e.g., the nonlinear transport through interacting nanosystems [8], the electric-field induced breakdown of the Mott insulator [5, 9], or Bloch oscillations [7, 10]. In most cases, theoretical predictions for the real-time response can be formulated only on the basis of numerical studies.

It is understood that for a weak driving force, the real-time response is determined by the equilibrium correlation functions as described by the linear-response (LR) theory. This theory has recently been extended to account for a system, that was previously driven out of equilibrium [11]. Furtheron we focus on the case of the charge current $I(t)$ in a one-dimensional (1D) system as induced by electric field $F(t)$, whereby the relevant equilibrium LR function is the dynamical conductivity $\sigma(\omega)$. For a generic (non-integrable) system of interacting (correlated) fermions at finite temperature $T > 0$ one expects within the LR regime the relaxation of current due to (Umklapp) scattering processes and hence finite d.c. value $\sigma_0 = \sigma(0)$. This, in turn, leads to a steady current under a constant driving field F . In contrast, it has been recognized that integrable systems in spite of interaction reveal a dissipationless component of the current response even at $T > 0$ as manifested by a finite charge

stiffness $D(T > 0) > 0$ [12]. Hence, the qualitative difference between both types of systems is expected to remain even for the nonlinear transport.

In this Letter, we address two aspects of the nonlinear transport in an isolated system of interacting tight-binding fermions under a time-dependent driving force: (i) How to generalize the LR response approach of generic systems at $T > 0$ to stronger fields and longer steady driving? Here we show that the dominating lowest-order mechanism beyond the LR regime is the increase of internal system energy or Joule-type heating (although we are not dealing with relaxation to canonical equilibrium) proportional to the square of the electric field. It could be accounted for by renormalization of the kinetic energy (as the sum rule for $\sigma(\omega)$ and, consequently the relevant σ_0). This extension allows one to predict strongly nonlinear response *without explicit solution* of the von Neumann or the time-dependent Schrödinger equations. (ii) Is there a qualitative difference in nonlinear response between integrable and non-integrable systems? Our results reveal a clear distinction between both categories whereby the response of integrable system to a steady field $F(t > 0) = \text{const}$ resembles the (damped) Bloch oscillations of noninteracting (NI) fermions, however, with nontrivially modified oscillation frequency.

We investigate an isolated 1D system of charged spinless fermions with periodic boundary conditions. The system is threaded by a time-dependent magnetic flux $\phi(t)$ and we assume that the flux enters only the kinetic energy term H_k of the Hamiltonian H

$$H = H_k + H_I, \\ H_k = -t_h \sum_j \left\{ e^{i\phi(t)} c_{j+1}^\dagger c_j + \text{h.c.} \right\}, \quad (1)$$

where $\phi = \tilde{\phi}/L$ is the flux per bond, L is the number of sites and H_I is assumed to be flux independent. We put furtheron $t_h = 1$. The time-dependent flux induces an electric field $F = -\dot{\phi}$. The charge current operator can

be written as

$$J = -\frac{\partial H}{\partial \phi} = \frac{i}{L} \sum_j \left\{ e^{i\phi(t)} c_{j+1}^\dagger c_j - \text{h.c.} \right\}. \quad (2)$$

Before specifying a particular form of the interaction term H_I and discussing numerical results it is instructive to derive simple equations of motion for the total energy $E(t) = \langle H(t) \rangle = \text{Tr}[\rho(t)H(t)]$, the kinetic energy $E_k(t) = \langle H_k(t) \rangle$ and the current $I(t) = \langle J(t) \rangle$. Making use of the von Neumann equation $i\dot{\rho}(t) = [H(t), \rho(t)]$ one can easily find the relations

$$\begin{aligned} \dot{E}(t) &= -i\text{Tr} \{ [H(t), \rho(t)] H(t) \} + \dot{\phi}(t) \text{Tr} \left[\rho(t) \frac{\partial H}{\partial \phi} \right] \\ &= L F(t) I(t), \end{aligned} \quad (3)$$

$$\dot{E}_k(t) = i\langle [H(t), H_k(t)] \rangle + L F(t) I(t), \quad (4)$$

$$\dot{I}(t) = i\langle [H(t), J(t)] \rangle - F(t) \frac{E_k(t)}{L}. \quad (5)$$

In the case of NI fermions $H_I = 0$, $H = H_k$ and commutators in Eqs. (4-5) vanish. Then, for a constant electric field $F(t) = F$ equations lead to harmonic oscillations with a frequency $\omega_B = F$, the solution known as Bloch oscillations.

Eq. (5) offers also a nontrivial approach to the nonlinear inverse problem, i.e., for arbitrary interaction term H_I one can find the tuning of the electric pulse $F(t)$ so that the induced current follows required time profile $I_a(t)$. Namely, putting $I_a(t)$ in the lhs. of Eq. (5) one can solve the equation for $F(t)$. This value of $F(t)$ determines the magnetic flux that should be used in the subsequent time step of the numerical solution of the von Neumann equation. Numerical results based on this method will be presented elsewhere.

In the following we study numerically the real-time current response within the 1D $t-V-W$ model,

$$H_I = V \sum_j \hat{n}_j \hat{n}_{j+1} + W \sum_j \hat{n}_j \hat{n}_{j+2}, \quad (6)$$

where $\hat{n}_j = c_j^\dagger c_j$, whereas V and W are (repulsive) interactions among particles on the nearest-neighbor and next-nearest-neighbor sites, respectively. In the absence of the external field the $t-V$ ($W=0$) model is integrable and within the LR theory $\sigma(\omega)$ has anomalous properties [12]. In particular, it can show a dissipationless component even at $T > 0$, i.e. $\sigma(\omega \sim 0) = D(T)\delta(\omega)$. $W \neq 0$ breaks the integrability leading to a finite d.c. $\sigma_0(T > 0) < \infty$ [12]. In the following we focus on the *metallic* regime of the half-filled systems with $n = N_e/L = 1/2$ and $V < 2t_h$.

Our aim is to study primarily a generic situation at $T > 0$ to avoid more specific cases emerging from the ground state. We perform the numerical evolution of the many-fermion wavefunction $|\Psi_l(t)\rangle$. The initial $|\Psi_l(0)\rangle$

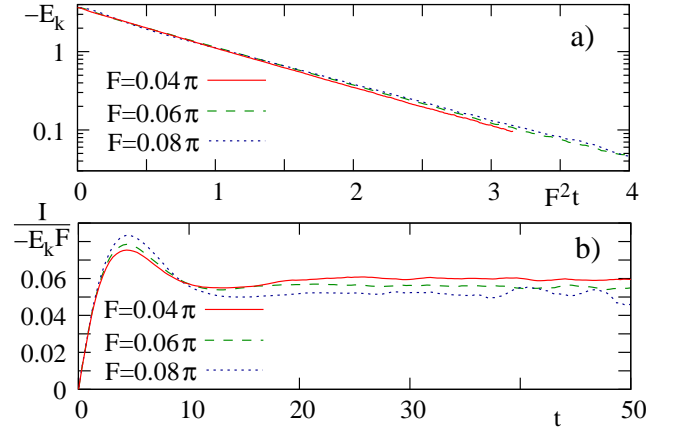


FIG. 1: (Color online) Real-time response: a) the kinetic energy $E_k(t)$, and b) the renormalized current $I(t)/(E_k(t)F)$ obtained for $N = 26$, $V = 1.4$ and $W = 1$. The electric field F is switched on at $t = 0$ and kept constant for $t > 0$.

should in principle be chosen as eigenstates of $H(0)$ distributed according to the canonical ensemble. Since the latter approach is possible only via full ED (typically $L < 16$ for the problem under consideration), we instead work using the microcanonical Lanczos method (MCLM) [13] allowing systems up to $L = 26$. First, we numerically generate approximate $|\Psi_l(0)\rangle$, $l = 1, N_s$ with energy $E(0) = \langle H(0) \rangle$ corresponding to the canonical value for given T (and L), but as well with a small energy uncertainty $\delta^2 E = \langle [H(0) - E(0)]^2 \rangle$. The time evolution $|\Psi_l(t)\rangle$ is then calculated by step-wise change of $\phi(t)$ in small time increments $\delta t \ll 1$ employing at each step Lanczos basis (typically $N_L = 10$) generating the evolution $|\Psi_l(t - \delta t)\rangle \rightarrow |\Psi_l(t)\rangle$. The described procedure is very robust and can be easily tested by changing $N_s, \delta E, \delta t$. In the following examples we study rather universal (but nontrivial) regime of quite elevated $T \sim 5$ where we use $N_s = 10, \delta E = 0.01, \delta t = 0.01$. Note that for systems considered ($L = 26$) number of basis states is typically $N_{st} \sim 10^7$ so that δE is still much bigger than the average level distance.

Let us start with the analysis of the non-integrable case where we take $V = 1.4$ and $W = 1$. For such choice of parameters LR $\sigma(\omega)$ [12] is rather featureless, i.e. broad in ω and, therefore, we may expect that numerical results are free of artifacts originating from some peculiar features of $\sigma(\omega)$. Fig. 1 shows the time dependence of the kinetic energy $E_k(t)$ (panel a) and the renormalized current $I(t)/[E_k(t)F]$ (panel b) for a system driven by a constant field $F(t > 0) = F$. One can see that $-E_k(t)$ goes exponentially to zero with the decay rate $\propto F^2$ and that the ratio $I(t)/[E_k(t)F]$ is almost constant for longer t . The dominating nonlinear effect thus consists in the increase of E_k . Since the latter also represents the sum rule, $\int \sigma(\omega) d\omega \propto |E_k|$, we formulate and test the following conjecture: $I(t)$ may be well approximated by the LR

theory extended to account for the increase of $E_k(t)$,

$$I(t) \simeq I_{\text{ER}}(t) = \frac{E_k(t)}{E_k(0)} I_{\text{LR}}(t), \quad (7)$$

$$I_{\text{LR}}(t) = \int_0^t dt' \sigma(t-t') F(t'), \quad (8)$$

where the conductivity response $\sigma(t-t')$ (evaluated from $\sigma(\omega)$) and consequently $I_{\text{LR}}(t)$ are determined within initial equilibrium state. Eq. (7) alone does not allow one to predict the real-time response without solving the time-dependent Schrödinger equation, since $E_k(t)$ is still needed. Although not fully evident, the accurate scaling presented in Fig. 1a together with Eqs. (3) and (7) indicate that the increase of E_k is just proportional to the increase of the total energy

$$\dot{E}_k(t) = \gamma \dot{E}(t) = \gamma L F I_{\text{ER}}(t). \quad (9)$$

Therefore, in the long-time regime of a driving with $F(t) = F$ one obtains $I_{\text{ER}}(t) = \sigma_0 F E_k(t)/E_k(0)$ and, consequently, $-E_k(t) \propto \exp(-\alpha F^2 t)$ with $\alpha > 0$. The coefficient γ is independent of F and can be estimated from the initial equilibrium state,

$$\gamma = \frac{E_k(t) - E_k(0)}{E(t) - E(0)} \simeq \frac{\partial E_k(0)}{\partial T} \left(\frac{\partial E(0)}{\partial T} \right)^{-1}. \quad (10)$$

The set of equations (7-10) fully determines $I_{\text{ER}}(t)$. Therefore, similarly to the LR theory, the real-time response can be calculated without explicit solution of the time-dependent problem. From the numerical point of view, these equations are not more demanding than the LR theory, as the only extension consists in the differential equation (9). In Fig. 2 we show the accuracy of the approximation given by Eq. (7). This figure demonstrates also the significance of the increase of total energy or Joule heating as the dominating nonlinear mechanism. Here, the value of γ has been determined from full diagonalization of a 10-site Hamiltonian.

We now turn our attention to the real-time response of an integrable interacting system, i.e. $W = 0$ case, where the above extension of the LR theory clearly breaks down. Now, a relevant reference is the NI $V = 0$ system, where for $F(t) = F$ current and the kinetic energy exhibit Bloch oscillations with $\omega_B = F$. It is expected that even at $V > 0$ a dissipationless component of current will retain the similarity to a NI system. We present in the following numerical results for the integrable metallic case $V = 1, W = 0$, where D (at $T \rightarrow \infty$) covers approximately half of the total spectral weight of $\sigma(\omega)$.

Inset in Fig. 3 shows $I(\phi)$ with $\phi = -Ft$ for the integrable t - V system driven by a constant electric field F . Contrary to the previously discussed $W \neq 0$ case, one observes a strong oscillatory behavior. For large enough $F > F^* \sim 0.5$, the frequency of the current oscillations ω (evaluated here from the second maximum of $I(t)$) is

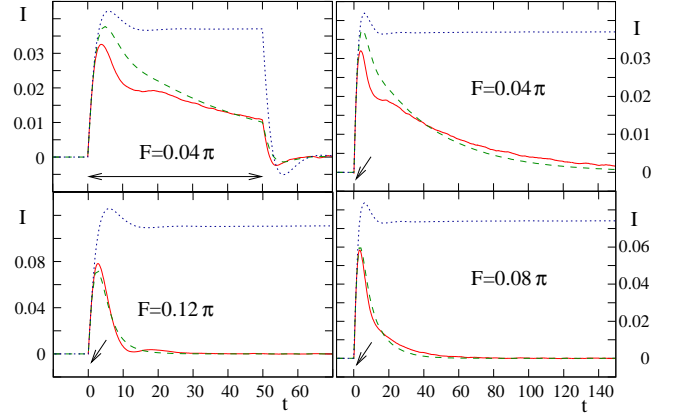


FIG. 2: (Color online) $I(t)$ for $N = 26$, $V = 1.4$ and $W = 1$. Arrows indicate the instants of time, when the electric field is switched on (all panels) and off (upper left panel). Full lines represent results obtained via unrestricted numerical solution, whereas dotted and dashed lines show approximate results of the LR theory, $I_{\text{LR}}(t)$, and the extended LR approach, $I_{\text{ER}}(t)$, respectively.

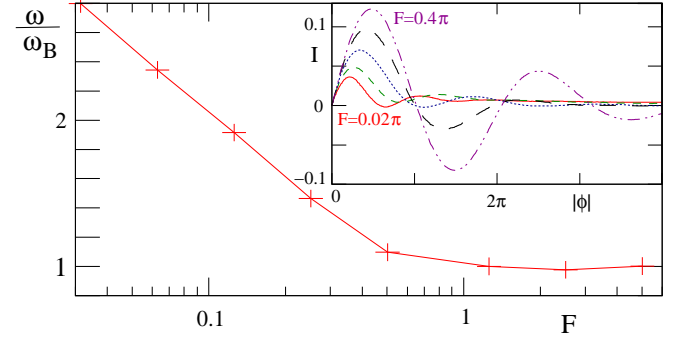


FIG. 3: (Color online) Current-oscillation frequency ω vs. field F normalized to ω_B of NI fermions, evaluated for $N = 26$, $V = 1, W = 0$. Inset: I vs. flux $|\phi|$ for different $F/\pi = 0.02, 0.04, 0.08, 0.16, 0.4$.

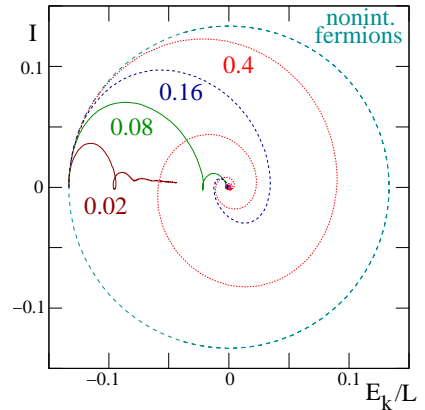


FIG. 4: (Color online) Relation between current $I(t)$ and kinetic energy density $E_k(t)/L$ for parameters as in Fig. 3, for different fields $F/\pi = 0.02 - 0.4$. Shown is also the results for NI fermions. The point and the arrow mark the initial state and the direction of evolution, respectively.

approximately the same as ω_B of NI fermions. Similar prediction has been obtained within nDMFT (see the discussion of a metallic phase in Ref. [7]). However, in the regime of a low electric fields $F < F^*$, the correlated system oscillates faster than ω_B . Within the investigated t - V model, ω/ω_B is found to increase *logarithmically* when the electric field decreases (see Fig. 3). The effect is present also for other $V < 2t_h$ although evidently the logarithmic regime disappears for $V \rightarrow 0$ where the NI universality sets in, i.e. in this case the crossover also moves to $F^* \rightarrow 0$.

At present we are unable to provide a physical explanation for the enhancement of ω/ω_B or to predict whether the logarithmic scaling breaks down for very low F . At least it is evident that $F > F^*$ response is similar to NI fermions in that both $I(t)$ and $E_k(t) = E(t)$ change sign during the evolution (see Fig. 4). On the contrary, the kinetic energy remains negative in the weak-field regime.

Still, for sufficiently short times of driving $t > 0$ the system's state is almost the initial one, i.e. $\rho(t) \simeq \rho(0)$, and the changes of $I(t)$ and $E_k(t)$ come from their explicit flux dependencies in Eqs. (1-2). Then, one can easily find from Eqs. (4-5) that $[E_k(t)]^2 + [LI(t)]^2 \simeq [E_k(0)]^2$, independently of the form of interaction term H_I . It explains, why the initial response as well as the strong-field response of a correlated system are the same as the response of NI fermions [14]. Moreover, assuming that the $E_k(t)$ and $I(t)$ do not cross the outer circle in Fig. 4 (what holds true in all investigated cases), one finds that the magnitude of current is bounded from above by the initial kinetic energy.

In conclusion, our study reveals several novel features of isolated interacting fermionic systems under constant or time-dependent driving force. For a generic system of tight-binding electrons we present a simple extension of the LR theory taking into account the change of kinetic energy. This approach gives a very satisfactory description of numerical results, at least for high enough T . Here, the basic condition is that in spite of driving, the system at all times satisfies the quasi-equilibrium relation between the kinetic energy $E_k(t)$ and the total energy $E(t)$. It seems plausible that the necessary condition for such a development is (fast enough) relaxation of current, here due to the Umklapp processes. It remains to be investigated whether a similar behavior applies to interacting systems beyond the tight-binding description (when e.g. the sum rule for $\sigma(\omega)$ is not directly E_k) or in low T regime. In the latter case the linear dependence $\dot{E}_k(t) \propto \dot{E}(t)$ should probably be replaced with a more general one $E_k(t) = E_k[E(t)]$.

On the other hand, integrable systems show strikingly different development. To first approximation the current $I(t)$ under constant driving reveals oscillations with the dominant dependence only on the flux $\phi(t)$. While

at large $F > F^*$ this has clear connection to the Bloch oscillations of tight-binding electrons with characteristic $\omega \sim \omega_B$, the effective ω is increasing for lower $F < F^*$ while at the same time oscillations are becoming damped (in fact the damping is found to be strongest at $F \sim F^*$). One part of this phenomena, in particular the damping, can be attributed to the breaking of integrability by introducing time-dependent $\phi(t)$. Oscillations themselves in the *low-field regime* are the signature of a coherent behavior which has to be intimately related to finite charge stiffness $D(T > 0) > 0$ since they disappear outside the metallic regime, e.g. for $V > 2t_h$ at half-filling $n = 1/2$. Alternatively, if the field is switched off in this regime before reaching $E_k \sim 0$ then the current relaxes to a finite $I(t = \infty) > 0$ being a direct consequence of $D(T > 0) > 0$. In any case, the observed phenomena reveal that even in weak fields the response of (near)integrable systems is far from the one expected from the equilibrium LR theory, but at the same time quite universal representing an open challenge for a proper explanation and also possible experimental observation.

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